

# Two- and three-body calculations within the dominantly orbital state method

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## Abstract

The dominantly orbital state method allows a semiclassical description of quantum systems and is expected to be valid for large values of the orbital angular momentum and small radial excitations. At the origin, it was developed for two-body relativistic systems. Here, the method is extended to treat two- and three-body Hamiltonians in  $D \geq 2$  dimensions with arbitrary kinetic energy and potential. It is shown that this method can produce quite accurate results, in some cases for the whole spectrum.

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## I. INTRODUCTION

The dominantly orbital state (DOS) method is a technique to compute approximate solutions for quantum eigenvalue problems [1]. The first step is to compute the energy associated with a classical circular motion and then quantize the orbital angular momentum. This kind of semiclassical approximation is expected to be valid only for high values of this quantum number. Then, the radial motion is quantized around the physical circular orbit. This implies that the radial excitation must be small compared to the orbital excitation. As it will be shown, this method is very simple to implement. The only mathematical difficulty is the computation of the physical radius which is the solution of a transcendental equation. In favorable cases, the solution can be analytical.

At the origin, the method has been developed for two-body relativistic Hamiltonians [1] and has been used to study hadronic systems [1–3]. The purpose of this work is to generalize this technique to treat two- and three-body Hamiltonians in  $D \geq 2$  spatial dimensions with arbitrary kinetic energy and potential. This is motivated by the existence of non-standard kinetic energies in some physical problems, for instance in atomic physics with non-parabolic dispersion relation [4], in hadronic physics with particle masses depending on the relative momentum [5], or in quantum mechanics with a minimal length [6, 7]. Moreover, problems in  $D$  dimensions can appear in various physical situations. In particular,  $D = 2$  systems can be used as toy models for  $D = 3$  systems [8] or are the natural framework for the physics of anyons [9]. Three-body calculations are much more involved than two-body ones. The purpose of the extension of the DOS method to this kind of calculations is not to compete with numerical methods such that expansions in harmonic oscillator basis [10] or in Gaussian states [11], but to provide rapidly approximate but reliable, and even analytical, results.

This paper is organized as follows. Some elements for the physics in  $D$  dimensions are briefly reminded in Sec. II. The DOS method for two-body systems is generalized in Sec. III to  $D$ -dimensional cases, and it is developed for three-body systems in Sec. IV. In both sections, applications are given to test the validity of the method. Concluding remarks are given in Sec. V.

## II. KINEMATICS IN $D$ DIMENSIONS

Let  $\mathbf{p}$  and  $\mathbf{r}$  be conjugate variables, then the operator  $\mathbf{p}^2$  in  $D \geq 2$  dimensions can be written as [12]

$$\mathbf{p}^2 = p_r^2 + \frac{\hat{\lambda}^2}{r^2} \quad \text{where} \quad p_r^2 = - \left( \frac{d^2}{dr^2} + \frac{D-1}{r} \frac{d}{dr} \right), \quad (1)$$

and where the orbital operator  $\hat{\lambda}^2$  is such that [13]

$$\hat{\lambda}^2 Y_{l,\{\mu\}}(\Omega_D) = l(l + D - 2) Y_{l,\{\mu\}}(\Omega_D). \quad (2)$$

Functions  $Y_{l,\{\mu\}}(\Omega_D)$  are hyperspherical harmonics on the  $D$ -sphere with spherical coordinates  $\Omega_D$ .  $l$  is the orbital quantum number and  $\{\mu\}$  are the magnetic quantum numbers. In semiclassical calculations, it is usual to replace the orbital factor  $l(l + a)$  by  $(l + b)^2$ , the two forms being equivalent for  $l \gg 1$ , that is to say a domain of values for which the semiclassical approximation is expected to be relevant. In this case, we have

$$\mathbf{p}^2 = p_r^2 + \frac{\lambda^2}{r^2} \quad \text{with} \quad \lambda = l + \frac{D-2}{2}. \quad (3)$$

## III. TWO-BODY SYSTEMS

### A. General formula

Let us consider the two-body Hamiltonian ( $\hbar = c = 1$ )

$$H = T(p) + V(r), \quad (4)$$

with  $p = |\mathbf{p}|$  and  $r = |\mathbf{r}|$ . For a circular motion ( $p_r = 0$ ), the semiclassical ( $\lambda$  is quantized) energy is given by

$$E(r) = T \left( \frac{\lambda}{r} \right) + V(r). \quad (5)$$

As usual, we assume that the physical orbit is determined by a minimum energy condition. This occurs for the radius  $r_0$  given by

$$\frac{\lambda}{r_0} T' \left( \frac{\lambda}{r_0} \right) = r_0 V'(r_0). \quad (6)$$

This condition has a natural explanation in terms of a centripetal force derived from a potential [14]. It is also a semiclassical version of the generalized virial theorem [15], as remarked in [16]. The corresponding energy is  $E_0 = E(r_0)$ .

In order to compute the radial excitation, we will quantize the radial motion  $\Delta r$  around a circular orbit with a fixed radius  $r_0 = r - \Delta r$ . This motion is controlled by the Hamiltonian

$$\Delta H = T \left( \sqrt{p_r^2 + \frac{\lambda^2}{(r_0 + \Delta r)^2}} \right) + V(r_0 + \Delta r) - E_0 \quad (7)$$

For small values of the radial quantum number  $n$ , we can expand  $\Delta H$  in powers of  $p_r^2$  and  $\Delta r$ . Keeping only the first non vanishing contributions, we obtain

$$\Delta H \approx \frac{1}{2\mu} p_r^2 + \frac{k}{2} \Delta r^2 \quad (8)$$

with

$$\mu = \frac{\lambda}{r_0 T' \left( \frac{\lambda}{r_0} \right)} \quad \text{and} \quad k = \frac{\lambda}{r_0^4} \left( 2 r_0 T' \left( \frac{\lambda}{r_0} \right) + \lambda T'' \left( \frac{\lambda}{r_0} \right) \right) + V''(r_0). \quad (9)$$

The term in  $\Delta r$  is canceled by the circular condition for the orbit. Since  $l \gg 1$ , the radius  $r$  is expected to be large. Under this condition, we can assume that  $p_r^2 \approx -d^2/dr^2$ , and  $\Delta H$  reduces to a one-dimensional harmonic oscillator whose eigenvalues are given by  $\Delta E = \sqrt{\frac{k}{\mu}} \left( n + \frac{1}{2} \right)$ . Finally, the total energy,  $E = E_0 + \Delta E$ , can be written

$$E = T \left( \frac{\lambda}{r_0} \right) + V(r_0) + \sqrt{\frac{2}{r_0^2} T' \left( \frac{\lambda}{r_0} \right)^2 + \frac{\lambda}{r_0^3} T' \left( \frac{\lambda}{r_0} \right) T'' \left( \frac{\lambda}{r_0} \right) + \frac{r_0}{\lambda} T' \left( \frac{\lambda}{r_0} \right) V''(r_0)} \left( n + \frac{1}{2} \right) \\ \text{with} \quad \frac{\lambda}{r_0^2} T' \left( \frac{\lambda}{r_0} \right) = V'(r_0) \quad \text{and} \quad \lambda = l + \frac{D-2}{2}. \quad (10)$$

This system is expected to be valid when  $l \gg 1$  and  $n \ll l$ . The relevance of this formulation is tested in Sec. III C for three analytical solutions of (10).

### B. Case $D = 2$ and $l = 0$

In the particular case  $D = 2$  and  $l = 0$ ,  $\lambda = 0$  and the system (10) is ill-defined. In principle, this is not a problem since the approximation is only valid for  $l \gg 1$ . Nevertheless, for some systems, it is possible to obtain a good accuracy even for small values of  $l$  (see following section). If the determination of  $r_0$  is analytical, a generic value of  $\lambda$  can be kept through the calculations. In the final formula, one must then check that the limit  $\lambda \rightarrow 0$  is relevant. If only numerical calculations are possible to fix  $r_0$ , it is then interesting to dispose of an alternative method to treat specifically the case  $\lambda = 0$ .

The WKB method is a powerful one to solve eigenequations without centrifugal term [17]. With our notation, the eigenvalue  $E$  can be computed by solving the following equation

$$2 \int_0^{r_*} T^{-1}(E - V(r)) dr = a n + b, \quad (11)$$

where  $a$  and  $b$  are two constants. With a vanishing orbital momentum for  $D = 2$  ( $\lambda = 0$ ), the classical motion runs from 0 to the turning point  $r_*$  given by

$$r_* = V^{-1}(E - T(0)). \quad (12)$$

We can fix  $a$  and  $b$  in order that the WKB solution gives the exact result for the harmonic oscillator. We have then

$$\int_0^{V^{-1}(E-T(0))} T^{-1}(E - V(r)) dr = \pi \left( n + \frac{1}{2} \right). \quad (13)$$

Equations (10) and (13) allow a determination of the energy spectrum for any value of  $\lambda$ .

### C. Applications

For the  $D$ -dimensional nonrelativistic harmonic oscillator,  $T(p) = p^2/(2m)$  and  $V(r) = k r^2/2$ , the system (10) gives

$$E = \sqrt{\frac{k}{m}} \left( 2n + l + \frac{D}{2} \right), \quad (14)$$

which is the exact result [12]. By construction, this result is also obtained by (13) for  $D = 2$  and  $l = 0$ .

For the  $D$ -dimensional Coulomb problem,  $T(p) = p^2/(2m)$  and  $V(r) = -\alpha/r$ , the system (10) gives

$$E = -\frac{m \alpha^2}{2 \left( l + \frac{D-2}{2} \right)^2} + \frac{m \alpha^2}{\left( l + \frac{D-2}{2} \right)^3} \left( n + \frac{1}{2} \right), \quad (15)$$

which are the first terms of the expansion of the exact solution [12]

$$E_{\text{exact}} = -\frac{m \alpha^2}{2 \left( n + l + \frac{D-1}{2} \right)^2} \quad (16)$$

for  $l \gg n$ . In the case  $D = 2$  and  $l = 0$ , (13) gives the exact result (16).

Let us now look at the following semirelativistic Hamiltonian

$$H = 2\sqrt{\mathbf{p}^2} + a r, \quad (17)$$

commonly used for the study of mesons composed of light quarks [18]. The eigenvalues of (17) are the masses of the system. An analytical solution of the system (10) can also be obtained in this case. As it is remarked in [1] for the case  $D = 3$ , a more accurate approximation is obtained by computing the square energy  $E^2$  but by dropping the term in  $(n + \frac{1}{2})^2$ , which is coherent with the DOS approximation. The final result is then

$$E^2 = 8a \left( \sqrt{2}n + l + \frac{D - 2 + \sqrt{2}}{2} \right). \quad (18)$$

The Hamiltonian (17) leads to Regge trajectories: The square mass is a linear function of  $l$  and  $n$  with slopes independent of  $D$ . The ratio between the radial and orbital slopes is  $\sqrt{2}$ , which is in agreement with the value  $\pi/2$  found in [19] for  $D = 3$  with a Bohr-Sommerfeld quantization procedure. For  $D = 2$  and  $l = 0$ , (13) gives

$$E^2 = 4\pi a \left( n + \frac{1}{2} \right), \quad (19)$$

which is in quite good agreement with (18). The accuracy of formula (18) is tested in table I for  $D = 3$ , where the DOS solutions are compared with the eigenvalues computed with the high accuracy numerical Lagrange-mesh method [20]. One can see that the agreement is very good, even for small values of  $l$  and large values of  $n$ . It is expected that the method be more accurate for Hamiltonians close to the harmonic oscillator one, whose spectrum is exactly reproduced.

## IV. THREE-BODY SYSTEMS

### A. General formula

Let us now consider a classical Hamiltonian for three identical particles interacting via the one-body  $U$  and two-body  $V$  interactions

$$H = \sum_{i=1}^3 T(|\mathbf{p}_i|) + \sum_{i=1}^3 U(|\mathbf{r}_i - \mathbf{R}|) + \sum_{i \leq j=1}^3 V(|\mathbf{r}_i - \mathbf{r}_j|), \quad (20)$$

where  $\sum_{i=1}^3 \mathbf{p}_i = \mathbf{0}$  and  $\mathbf{R} = \frac{1}{3} \sum_{i=1}^3 \mathbf{r}_i$  is the center of mass position. A set of internal coordinates ( $\mathbf{x} = \mathbf{x}_1 = \mathbf{r}_1 - \mathbf{r}_2, \mathbf{x}_2 = \mathbf{r}_2 - \mathbf{r}_3, \mathbf{x}_3 = \mathbf{R}$ ) can be defined together with its conjugate variables ( $\mathbf{q} = \mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3$ ). In order to apply the DOS approximation, we will

TABLE I. Eigenmasses  $E/\sqrt{a}$  of the Hamiltonian (17) for  $D = 3$ . For each set of quantum numbers  $\{l, n\}$ , the first line is an accurate value obtained by the Lagrange-mesh method [20], and the second line is given by (18).

	$n = 0$	1	2	3
$l = 0$	3.157	4.709	5.889	6.871
	3.108	4.579	5.682	6.603
1	4.225	5.457	6.483	7.375
	4.202	5.382	6.347	7.183
2	5.079	6.130	7.047	7.867
	5.065	6.080	6.949	7.720
3	5.811	6.724	7.577	8.338
	5.801	6.706	7.502	8.222

impose a severe constraint on the system: the three particles move on a circular motion around the center of mass at the apex of an equilateral triangle. Under these conditions, we have  $x = |\mathbf{x}| = |\mathbf{r}_i - \mathbf{r}_j| = \sqrt{3} |\mathbf{r}_i - \mathbf{R}|$  and  $q = |\mathbf{q}| = |\mathbf{p}_i|$ ,  $\forall i$  and  $j$ . The Hamiltonian (20) can then be rewritten

$$H_{\text{DOS}} = 3 [T(q) + W(x)] \quad \text{with} \quad W(x) = U\left(\frac{x}{\sqrt{3}}\right) + V(x). \quad (21)$$

In this Hamiltonian,  $\mathbf{q}^2 = q_r^2 + \frac{\lambda^2}{x^2}$ .

In order to interpret correctly the quantum numbers associated with the conjugate variables  $\mathbf{x}$  and  $\mathbf{q}$ , once quantized, let us look at the total orbital angular momentum. In the center of mass frame, it is given by  $\mathbf{L} = \sum_{i=1}^3 (\mathbf{r}_i - \mathbf{R}) \times \mathbf{p}_i$ , and is such that

$$|\mathbf{L}| = \sqrt{3} |\mathbf{x} \times \mathbf{q}|. \quad (22)$$

If  $\Lambda$  ( $\lambda$ ) is the orbital angular momentum associated with  $\mathbf{L}$  ( $\mathbf{x} \times \mathbf{q}$ ), we have  $\Lambda = \sqrt{3} \lambda$ . Physically,  $\Lambda$  must be associated with the contributions brought by the two internal variables, and we can expect that  $\Lambda = (l_1 + \frac{D-2}{2}) + (l_2 + \frac{D-2}{2})$ , where  $l_1$  and  $l_2$  are the orbital angular momentums associated with these variables. Finally, we identify

$$\lambda = \frac{1}{\sqrt{3}} (L + D - 2) \quad \text{with} \quad L = l_1 + l_2. \quad (23)$$

In a semiclassical approach, the quantification of the radial motion for the three-body system is given by the integral of the quantity  $3 p_r \Delta r$ , where  $p_r$  is the radial momentum for one particle and  $\Delta r$  is the variation of the radius of the circular motion. We have  $3 p_r \Delta r = \sqrt{3} q_r \Delta x$ , where  $q_r$  and  $\Delta x$  are the equivalent quantities for the variables  $\mathbf{q}$  and  $\mathbf{x}$ . If  $\nu (n + 1/2)$  is the radial quantum factor associated with  $3 p_r \Delta r$  ( $q_r \Delta x$ ), we have  $\nu = \sqrt{3}(n + 1/2)$ . Physically,  $\nu$  must be associated with the contributions brought by the two internal variables, and we can expect that  $\nu = (n_1 + \frac{1}{2}) + (n_2 + \frac{1}{2})$ , where  $n_1$  and  $n_2$  are the radial quantum numbers associated with these variables. Finally, we identify

$$n + \frac{1}{2} = \frac{N + 1}{\sqrt{3}} \quad \text{with} \quad N = n_1 + n_2. \quad (24)$$

Using the same procedure as in Sec. III A, we can find the DOS solution for (21). It is written

$$\frac{E}{3} = T\left(\frac{\lambda}{x_0}\right) + W(x_0) + \sqrt{\frac{2}{x_0^2} T'\left(\frac{\lambda}{x_0}\right)^2 + \frac{\lambda}{x_0^3} T'\left(\frac{\lambda}{x_0}\right) T''\left(\frac{\lambda}{x_0}\right) + \frac{x_0}{\lambda} T'\left(\frac{\lambda}{x_0}\right) W''(x_0)} \frac{N + 1}{\sqrt{3}}$$

with  $\frac{\lambda}{x_0^2} T'\left(\frac{\lambda}{x_0}\right) = W'(x_0)$  and  $\lambda = \frac{1}{\sqrt{3}}(L + D - 2)$ . (25)

Again, this system is expected to be valid when  $L \gg 1$  and  $N \ll L$ . The relevance of this formulation is tested in Sec. IV C for two analytical solutions of (25).

If the masses of the three bodies are different, the assumption  $|\mathbf{q}| = |\mathbf{p}_i|$  is no longer justified. So, the present approximation scheme should not be applied. However, if a strong mass asymmetry exists between the particles, the problem can be reduced to a two- or one-body problem thanks to an adiabatic approximation.

### B. Case $D = 2$ and $L = 0$

Again, if  $D = 2$  and  $L = 0$ , the system (25) is no longer well-defined. Using, the same considerations as in Sec. III B, the WKB method can be used to treat this particular case. This finally gives

$$\int_0^{W^{-1}\left(\frac{E}{3} - T(0)\right)} T^{-1}\left(\frac{E}{3} - W(x)\right) dx = \frac{\pi}{\sqrt{3}}(N + 1). \quad (26)$$

From [21], it is easy to determine that the exact solution for the general nonrelativistic  $D$ -dimensional three-body harmonic oscillator,  $T(q) = q^2/(2m)$ ,  $U(x) = kx^2$  and  $V(x) = \rho x^2$ ,



is written

$$E = \sqrt{\frac{2}{m}(k + 3\rho)} (2n_1 + 2n_2 + l_1 + l_2 + D). \quad (27)$$

It can be checked that (26) gives the exact result with  $D = 2$ ,  $l_1 = l_2 = 0$ , and  $N = n_1 + n_2$ .

### C. Applications

For the general three-body harmonic oscillator defined in the previous section, the system (25) gives

$$E = \sqrt{\frac{2}{m}(k + 3\rho)} (2N + L + D). \quad (28)$$

which is the exact result with the identification  $N = n_1 + n_2$  and  $L = l_1 + l_2$ . This confirms the interpretation chosen for the quantum numbers  $N$  and  $L$  in Sec. IV A. By construction, this result is also obtained by (26) for  $D = 2$  and  $L = 0$ .

Let us now look at the following semirelativistic Hamiltonian

$$H = \sum_{i=1}^3 \sqrt{\mathbf{p}_i^2} + a \sum_{i=1}^3 |\mathbf{r}_i - \mathbf{R}| + b \sum_{i \leq j=1}^3 |\mathbf{r}_i - \mathbf{r}_j|, \quad (29)$$

used for the study of baryons composed of light quarks [22]. It can be seen as the three-body generalization of (17). The eigenvalues of (29) are the masses of the system. An analytical solution of the system (25) can also be obtained in this case. As for the two-body Hamiltonian, a more accurate approximation is obtained by computing the square energy  $E^2$  but by dropping the term in  $(N + 1)^2$ . The final result is then

$$E^2 = 12c \left( \sqrt{2}N + L + D - 2 + \sqrt{2} \right) \quad \text{with} \quad c = a + \sqrt{3}b. \quad (30)$$

By comparing this equation with (18), one can see that the same ratio between the Regge slopes is predicted for two- and three-body systems, as expected [23]. For  $D = 2$  and  $L = 0$ , (26) gives

$$E^2 = 6\pi c (N + 1), \quad (31)$$

which is in quite good agreement with (30).

The eigenstates of the Hamiltonian (29) have also been computed with a high accuracy method relying on the expansion of trial states on a harmonic oscillator basis [10]. The lowest eigenstates are characterized by a large component (generally more than 90%) spanned by one or several harmonic oscillator basis states with the same fixed value of  $N = n_1 + n_2$

and  $L = l_1 + l_2$ . So they can be labeled by the number of quanta  $Q = L + 2N$ , and the corresponding eigenvalues can be easily compared with the predictions of the DOS method. All eigenvalues for the completely symmetrical and the completely antisymmetrical states are presented in Fig. 1. For the clearness of the figure, only the eigenvalue corresponding to the mixed symmetry state for  $Q = 1$  is shown. One can see that the agreement is quite good, even if some degeneracies remain. In a pure harmonic oscillator picture, all masses associated with the same value of  $Q$  should be degenerate. It can be observed in Fig. 1 that the DOS spectrum reproduces energy levels with any symmetry at the quantum level. Actually,  $H_{\text{DOS}}$  and  $H$  are both symmetrical for the exchange of particles, but depends on less variables. Thus, the DOS method does not have enough degrees of freedom to study quantum states with a particular symmetries and the mass degeneracies due to quantum symmetries are not lifted.

The DOS method presented here shares some similarities with the envelope theory (or equivalently the auxiliary field method) [16, 21, 24, 25]. For vanishing radial excitations, both methods reduce to a similar set of equations: one to fix the energy as a function of a mean radius and the other to determine this radius from a transcendental equation. At the origin, the envelope theory was developed for  $D = 3$ . But, as it relies on the exact solutions for harmonic oscillator Hamiltonians, it is not difficult to extend it to any  $D$ . Within this framework, the prediction of the envelope theory for the eigenvalues of Hamiltonian (29) is [21]

$$E^2 = 12c(2N + L + D) = 12c(Q + D). \quad (32)$$

This formula is similar to (30). It is an upper bound, but it suffers from a strong degeneracy in  $Q = 2N + L$ . Formula (30) does not yield bounds on eigenvalues but finally produces better results, since it has the nice feature of lifting the harmonic oscillator degeneracy.

## V. CONCLUDING REMARKS

The dominantly orbital state (DOS) method is a semiclassical technique to compute approximate solutions for quantum eigenvalue problems [1]. It is expected to be valid only for high values of the orbital angular momentum and small radial excitations, but it can give good results for the whole spectra in some particular cases. This method is very simple to implement and needs only the solution of a transcendental equation. In favorable cases,

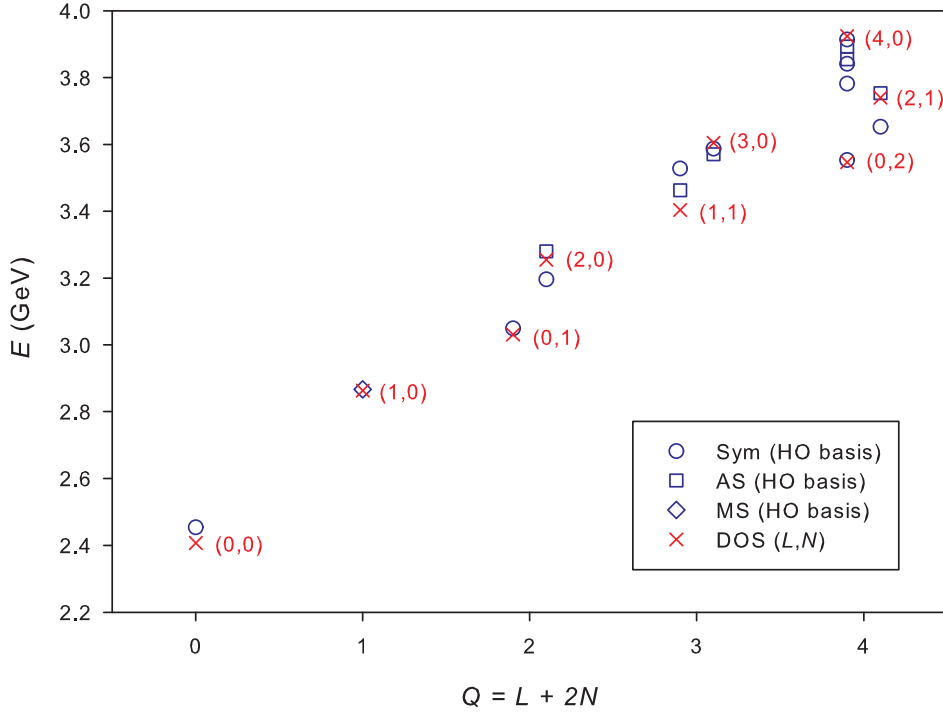


FIG. 1. Eigenmasses  $E$  in GeV of Hamiltonian (29) for  $D = 3$ , and for  $a = 0.2 \text{ GeV}^2$  and  $b = 0$ , as a function of the number of quanta  $Q$ , obtained by an accurate computation in a harmonic oscillator basis [10]: All values corresponding to completely symmetrical (circle) and completely antisymmetrical (square) states; Only the value corresponding to the mixed symmetry (diamond) state for  $Q = 1$ . The corresponding approximate values (cross) given by formula (30) are indicated with the quantum numbers  $(L, N)$ .

an analytical formula can be obtained.

Developed at the origin for two-body relativistic systems, it is extended here to treat two- and three-body Hamiltonians in  $D \geq 2$  dimensions with arbitrary kinetic energy and potential. A lot of accurate techniques exist to solve numerically two-body problems. So, the DOS method is specially interesting for cases in which it can produce an analytical solution. But, since quite good results can be obtained by the method, they can also be used to check a numerical procedure.

A three-body problem is always difficult to solve, and techniques to implement it can be very heavy [10, 11]. In this case, the purpose of the DOS method is not to compete with these very accurate techniques, but instead to provide rapidly approximate, and even

analytical, results. Despite the strong constraint imposed on the motion of the particles, the results obtained seem reliable: We reproduce the harmonic spectrum exactly and the Regge trajectories of relativistic systems with a linear confinement. An interesting feature of the DOS method is that it lifts the harmonic oscillator degeneracy which is present in other methods [16, 21, 24, 25]. This property can be particularly interesting when applied to hadronic physics for example [26]. Moreover the DOS method can also be used to check a – often complicated – numerical procedure.

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